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General Eigenvalue Solver for Large Sparse Symmetric Matrix with Zero Filtering

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A general eigenvalue solver for a large sparse symmetric matrix with zero eigenvalue solutions is developed using a subspace method. The technique for the large sparse system is a list vector; for a system with zero eigenvalues, a zero filter technique is added. The solutions can be obtained starting from the smallest eigenvalue excepting zero eigenvalue solutions.

KEY WORDS: Acceleration/ Eigenvalue/ ICCG/ Large sparse matrix/ Zero eigenvalue/ Zero filter/

1. INTRODUCTION

RF acceleration cavities have been evaluated by numerical computing methods as electro-magnetic eigenvalue problems. The usual methods are FEM (Finite Element Method), FDM (Finite Difference method) and so on. In those methods, field variables are chosen to express enough information about the electro-magnetic field. For example, only one component such as E_z is enough to represent two dimensional electromagnetic fields and the problem can be treated as a scalar potential problem. In these days, computing power is going up, and three dimensional problems are within reach; in these, three vector components must be used as field variables. But this introduces difficulties such as the spurious problem, where many spurious solutions which do not satisfy the zero-divergence condition appear in the series of eigen solutions. Recently, new techniques for FEM have been developed[1] to overcome these difficulties. They often use exotic elements satisfying the zero divergent condition of electric vector field $\boldsymbol{E}$, for which the basic equation in vacuum has to be

$$\nabla\times\nabla\times\boldsymbol{E}=\lambda\boldsymbol{E}, \tag{1}$$

where $\lambda=\omega^2/c^2$, $\omega=2\pi f$, f is the frequency and c is the speed of light. Often of interest are several solutions starting from the lowest frequency. Unfortunately, many of the lowest eigenvalues can be zero ($\nabla\times\nabla\times\boldsymbol{E}=0$) and normal iteration methods such as subspace methods cannot be applied without eigenvalue shift.

To avoid the problem, some times they use the relations

$$\Delta\boldsymbol{E}\equiv\nabla^2\boldsymbol{E}=\nabla(\nabla\cdot\boldsymbol{E})-\nabla\times\nabla\times\boldsymbol{E}, \tag{2}$$

and the equation becomes the vector wave equation

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$$\Delta \boldsymbol{E} = -\lambda \boldsymbol{E}, \tag{3}$$

but this formulation is not useful for exotic elements because the elements themselves satisfy $\nabla \cdot \boldsymbol{E} = 0$ and Eq. (1) and Eq. (3) are equivalent.

2. EIGENVALUE PROBLEM

Using FEM, the differential equation (1) can be expressed as a general eigenvalue problem in matrix form;

$$\boldsymbol{M} \cdot \boldsymbol{x} = \lambda \boldsymbol{K} \cdot \boldsymbol{x}, \tag{4}$$

where $\boldsymbol{M}$ is a non-negative-definite and $\boldsymbol{K}$ is a positive-definite sparse symmetric matrix of size N+1. Let Eq. (4) have the following solutions;

$$\boldsymbol{M} \cdot \boldsymbol{e}_i = \lambda_i \boldsymbol{K} \cdot \boldsymbol{e}_i, \tag{5}$$
$$(\lambda_i = 0;\ i = 0,\ 1,\ 2,\ \cdots\cdots l-1,\ \text{and}\ 0 < \lambda_l \leqq \lambda_{l+1} \leqq \cdots\cdots \leqq \lambda_N)$$

where $\boldsymbol{e}_i$ and λ_i are the i-th eigenvector and eigenvalue. This problem has l degenerated zero eigenvalue solutions. These zero eigenvalues make the normal subspace method inapplicable. The usual algorithm for a subspace method to get several solutions starting from smallest eigenvalues is as follows:[2, 3]

0) Take m initial vectors $\boldsymbol{X}$.
   (a column vector of $\boldsymbol{X}$ is one of m initial vectors $\boldsymbol{x}_i$.)
1) $\boldsymbol{Z} = \boldsymbol{K} \cdot \boldsymbol{X}$
2) $\boldsymbol{Y} = \boldsymbol{M}^{-1} \cdot \boldsymbol{Z}$
3) Transform to subspace,
   $\tilde{\boldsymbol{M}} = \boldsymbol{Y}^T \cdot \boldsymbol{M} \cdot \boldsymbol{Y}$ $(\tilde{\boldsymbol{M}} = \boldsymbol{Y}^T \cdot \boldsymbol{Z})$
   $\tilde{\boldsymbol{K}} = \boldsymbol{Y}^T \cdot \boldsymbol{K} \cdot \boldsymbol{Y}$
4) Solve the small eigenvalue problem $\tilde{\boldsymbol{M}} \cdot \boldsymbol{p} = d\, \tilde{\boldsymbol{K}} \cdot \boldsymbol{p}$
   and make $\boldsymbol{P} = [\boldsymbol{p}_1\ \boldsymbol{p}_2 \cdots \boldsymbol{p}_m]$.
5) Return to original space with $\boldsymbol{X} = \boldsymbol{Y} \cdot \boldsymbol{P}$, and normalize $\boldsymbol{x}_i$'s.

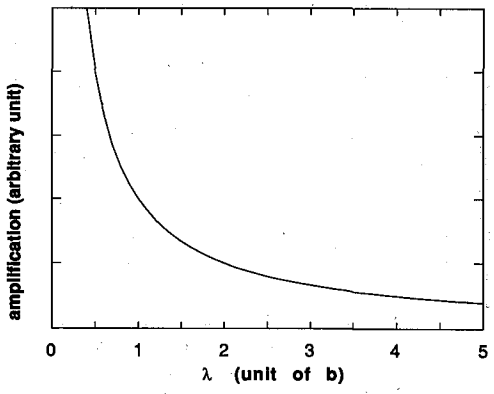

Fig. 1. The amplification of a component in each iteration as a function of the eigenvalue, for the usual subspace method.

6) If the solution has not converged, repeat from 1).
7) The d's are the eigenvalues and the column vectors of $\boldsymbol{X}$ are the eigenvectors.

In Fig. 1 the amplification of a component in each iteration is graphically shown as a function of the eigenvalue.

Having zero eigenvalue(s) makes $\boldsymbol{M}$ not regular, and step 2) is not possible (cannot solve with $\boldsymbol{M}$). In following section, a method to overcome the difficulty is described.

3. ZERO FILTER METHOD

Let $\boldsymbol{x}$ be an initial vector. Expand $\boldsymbol{x}$ with the eigen vectors of Eq. (1).

$$\boldsymbol{x}=\sum_{i=0}^{N} a_i \boldsymbol{e}_i. \tag{6}$$

Let $\boldsymbol{N}=\boldsymbol{M}+b\,\boldsymbol{K}$, where the shift value $b>0$. $\boldsymbol{N}$ is positive-definite. From Eq. (5), we get

$$\boldsymbol{N}\cdot\boldsymbol{e}_i=(\lambda_i+b)\,\boldsymbol{K}\cdot\boldsymbol{e}_i,\ (i=0,\ 1,\ \cdots N) \tag{7}$$

Eq. (5) multiplied by $\boldsymbol{N}^{-1}=(\boldsymbol{M}+b\boldsymbol{K})^{-1}$ from the left gives

$$\boldsymbol{e}_i=(\lambda_i+b)\,\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\cdot\boldsymbol{e}_i,\ (i=0,\ 1,\ \cdots N) \tag{8}$$

And we get

$$\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\cdot\boldsymbol{e}_i=\frac{1}{\lambda_i+b}\,\boldsymbol{e}_i \tag{9}$$

This operation is the basic amplification for one iteration of the subspace method. With only this operation, the solutions with largest amplification are those with zero eigenvalue. For Eq. (7), the zero eigenvalue is shifted to b. Let's think about the following operation

$$\frac{1}{b}-\boldsymbol{N}^{-1}\cdot\boldsymbol{K}. \tag{10}$$

Multiplying (10) by $\boldsymbol{x}$ and using Eq. (9), we get

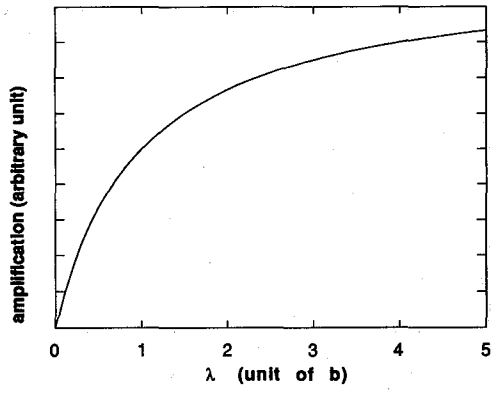

Fig. 2. The amplification of a component in each iteration as a function of the eigenvalue, for the zero filter.

$$\left(\frac{1}{\mathrm{b}}-\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\right)\boldsymbol{x}=\sum_{i=0}^{\mathrm{N}}\left(\frac{1}{\mathrm{b}}-\frac{1}{\lambda_{\mathrm{i}}+\mathrm{b}}\right)(\mathrm{a}_i\boldsymbol{e}_i). \tag{11}$$

Because $\lambda_{\mathrm{i}}=0$ for $\mathrm{i}<l$, Eq. (11) becomes

$$\left(\frac{1}{\mathrm{b}}-\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\right)\boldsymbol{x}=\sum_{i=l}^{\mathrm{N}}\left(\frac{1}{\mathrm{b}}-\frac{1}{\lambda_{\mathrm{i}}+\mathrm{b}}\right)(\mathrm{a}_i\boldsymbol{e}_i). \tag{12}$$

This means that the zero eigenvalue component vanishes with operation (11) within the precision of the "zero eigenvalue". Fig. 2 shows the schematic view of the idea. Let's call this operation "zero filter". Applying zero filter to the iterative procedure periodically, we can get the lowest several nonzero eigenvalues. The number of zero eigenvalues l does not matter. Applying zero filter to every iteration, the amplification of each component is

$$\left(\frac{1}{\mathrm{b}}-\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\right)\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\cdot\boldsymbol{x}=\sum_{i=l}^{\mathrm{N}}\frac{1}{\lambda_i+\mathrm{b}}\left(\frac{1}{\mathrm{b}}-\frac{1}{\lambda_{\mathrm{i}}+\mathrm{b}}\right)(\mathrm{a}_i\boldsymbol{e}_i). \tag{13}$$

Fig. 3 shows Eq. (13) graphically. The shift value b should be made about equal to λ_l for fast convergence in this case. The guess value for λ_l could be known from the physical characteristics of the problem.

If the zero eigenvalue precision is good enough, the filter may not have to be applied so frequently. Let ε_0 be the eigeuvalue with the worst error of the "zero" eigenvalues. Assuming that $\varepsilon_0 \ll \mathrm{b}$, the growth of the eigensolution component associated with ε_0 is, for each iteration,

$$\eta_0=\frac{1}{\varepsilon_0+\mathrm{b}}\simeq\frac{1}{\mathrm{b}}. \tag{14}$$

The error for each zero filter operation (the residual of zero eigen value component) is

$$\left(\frac{1}{\mathrm{b}}-\frac{1}{\varepsilon_0+\mathrm{b}}\right)\simeq\frac{\varepsilon_0}{\mathrm{b}^2}. \tag{15}$$

The amplitude for the zero eigensolution j times after the zero filter operation is order of

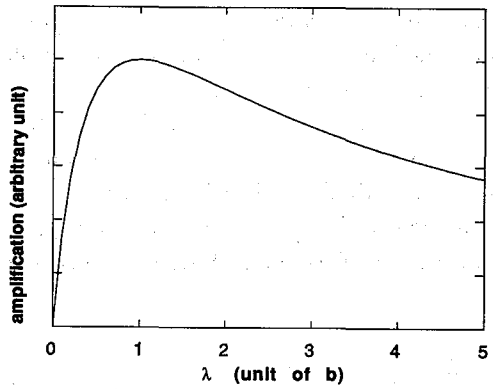

Fig. 3. The amplification as a function of the eigenvalue for the subspace method, with zero filter.

$$\frac{\varepsilon_0}{b^2}\left(\frac{1}{b}\right)^j. \tag{16}$$

The m-th eigensolution having the largest eigenvalue in those to be obtained has the smallest amplification;

$$\eta_m=\frac{1}{\lambda_{l+m}+b}. \tag{17}$$

The condition not to contaminate the largest eigenvalue solution so much with the zero-eigenvalue one is

$$\frac{1}{(\lambda_{l+m}+b)^j}\gg\frac{\varepsilon_0}{b^2}\left(\frac{1}{b}\right)^j. \tag{18}$$

From Eq. (18) we can find the periodicity j to apply the zero filter:

$$j<\frac{\log\left(\frac{b^2}{\varepsilon_0}\right)}{\log\left(\frac{\lambda_{l+m}+b}{b}\right)} \tag{19}$$

For example, assuming that $\varepsilon_0=10^{-4}$, $b=1$, and $\lambda_{l+m}=10\,b$, the condition is $j<4$. Finally, the algorithm is as follows;

0) Take m initial vectors $\boldsymbol{X}$.
   (a column vector of $\boldsymbol{X}$ is one of m initial vectors x_i.)
1) $\boldsymbol{N}=\boldsymbol{M}+b\boldsymbol{K}$
2) If needed, $\boldsymbol{Y}=\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\cdot\boldsymbol{X}$, $\boldsymbol{X}=\boldsymbol{X}-b\boldsymbol{Y}$ ⟵ ZERO FILTER
3) $\boldsymbol{Z}=\boldsymbol{K}\cdot\boldsymbol{X}$, $\boldsymbol{Y}=\boldsymbol{N}^{-1}\cdot\boldsymbol{Z}$
4) to 8) same as 3) to 7) of the subspace method procedure.

4. FILTER ACCELERATION METHOD

In an iterative method, the shift value b is sometimes taken to be negative and the eigenvalue of interest is shifted to around zero. Then the convergence is very fast because it is proportional to $1/(\lambda+b)$ and $b\simeq-\lambda$. Disadvantages are the following: 1) The matrix is not positive-definite. 2) The solutions are not obtained simultaneously starting from the lowest one.

With the zero filter method, b is positive and the matrix to be solved with is positive-definite, which is preferable for the iterative simultaneous equation solver method (particularly for CG method which will be stated later). However, positive b makes the eigenvalue covergence slower compared to the negative b method. We can also use the filter method as an acceleration technique to make convergence faster. The required operation is

$$\left(\boldsymbol{N}^{-1}\cdot\boldsymbol{K}-\frac{1}{c}\right)\boldsymbol{x}=\sum_{i=l}^{N}\left(\frac{1}{\lambda_i+b}-\frac{1}{c}\right)\cdot(a_i\boldsymbol{e}_i). \tag{20}$$

The schematic graph of Eq. (20) is shown in Fig. 4. In the figure, c is chosen to filter

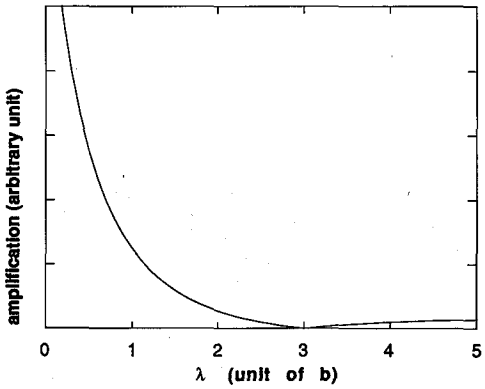

Fig. 4. The amplification as a function of the eigenvalue for the subspace method, with filter acceleration.

out the component of magnitude 3b, or c=4b. Applying this to every iteration with the zero filter, the amplification of each component is

$$\left(\boldsymbol{N}^{-1}\cdot\boldsymbol{K}-\frac{1}{\mathrm{c}}\right)\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\cdot\boldsymbol{x}=\sum_{i=l}^{\mathrm{N}}\frac{1}{\lambda_{\mathrm{i}}+\mathrm{b}}\left(\frac{1}{\lambda_{\mathrm{i}}+\mathrm{b}}-\frac{1}{\mathrm{c}}\right)\cdot(\mathrm{a}_i\boldsymbol{e}_i). \tag{21}$$

Fig. 5 shows Eq. (21) graphically. A local maximum point is at 2c−b. If the value of c is constant throughout the process, c should be about $1.2\times(\lambda_{l+\mathrm{m}+1}+\mathrm{b})$, because the amplification for the needed component should exceed that of the local maximum. Usually $\lambda_{l+\mathrm{m}+1}$ is not known a priori, then we first execute the procedure without acceleration. Eigenvalues settle faster than eigenvectors. The initial value of c is made to start about twice of the settled value of $(\lambda_{l+\mathrm{m}+1}+\mathrm{b})$. With each acceleration step, the value of c is decreased toward $1.2\times(\lambda_{l+\mathrm{m}+1}+\mathrm{b})$ step by step. One decrement method is to take an average between c and $1.2\times(\lambda_{l+\mathrm{m}+1}+\mathrm{b})$. It is a safe method because the eigenvalues converge from above, if the components of zero eigenvalue are suppressed to be small enough. Since mixtures of error happen to make the suppressed component bigger again, the value c has to go back to current $2\times(\lambda_{l+\mathrm{m}+1}+\mathrm{b})$ in some steps. The

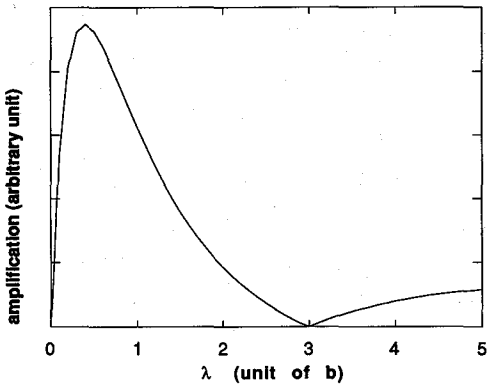

Fig. 5. The amplification as a function of the eigenvalue for the subspace method, with zero filter and filter acceleration.

final algorithm is as follows:

0) Take m initial vectors $\boldsymbol{X}$.
   (a column vector of $\boldsymbol{X}$ is one of m initial vectors x_i.)
1) $\boldsymbol{N}=\boldsymbol{M}+b\boldsymbol{K}$
2) Do either or neither of a) or b)
   a) $\boldsymbol{Y}=\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\cdot\boldsymbol{X}$, $\boldsymbol{X}=\boldsymbol{X}-b\boldsymbol{Y}$ ⟵ ZERO FILTER
   b) $\boldsymbol{Y}=\boldsymbol{N}^{-1}\cdot\boldsymbol{K}\cdot\boldsymbol{X}$, $\boldsymbol{X}=c\boldsymbol{Y}-\boldsymbol{X}$ ⟵ FILTER ACCELERATION
      and change c.
3) to 8): same as ZERO FILTER METHOD

5. STORAGE METHOD FOR LARGE SPARSE MATRIX

In FEM, the discretization may not be topologically regular; then the matrix structure is not regular. Conventional computer memory storage techniques were the band matrix storage which holds only the band part of constant width around the diagonal, or the skyline method which changes the width. The matrix size of a three dimensional problem was $\propto n^3$ and the band width was $\propto n^2$ where n is the number of mesh divisions on one axis. The storage requirement of both methods is $\propto n^5$. This number could easily explode if the mesh were made finer, although the actual number of non zero elements in the matrix is $\propto n^3$.

A list vector technique can be used which stores only the nonzero elements of the lower half of the matrix. The information structure is shown in Fig. 6. Array A holds the nonzero elements of M or K. INDEX (I) points to the left most element of I-th line of the matrix in array A. KOLUM(N) indicates the column number of A(N) element. In the general eigenvalue problem, there are two matrices and the required storage is

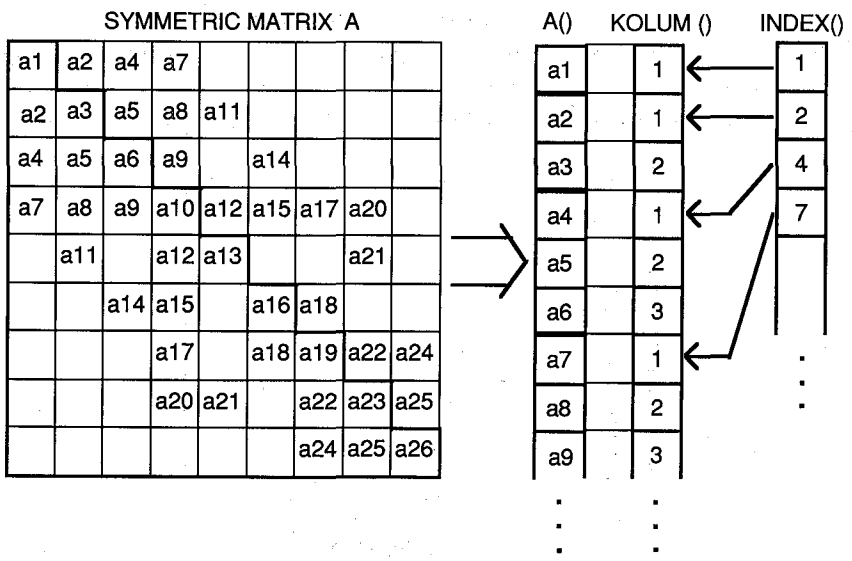

Fig. 6. A list vector technique stores only the nonzero elements of the lower half of the matrix. The information structure is shown.

$2\times e\times k\times 8\div 2$ bytes for double precision nonzero elements in M and K, $k\times 4$ bytes for INDEX, and $e\times k\times 4\div 2$ bytes for KOLUM, where e is the average number of coefficients connected to a component and k is the total variable number. A subroutine to prepare these INDEX and KOLUM information is supplied for user convenience.

The simultaneous equation solver used here is the ICCG method[4, 5], basically a Conjugate Gradient Method (CG method) with preconditioner. The preconditioner is given by the incomplete Cholesky decomposition. The current version has some room for modifications to reduce the iteration time. One is the modification to the incomplete Cholesky decomposition. Work on this subject will be reported separately.

6. DISCUSSION

With these techniques, we can get m eigen solutions starting from lowest frequency without any zero eigenvalue solution. The main cost (in terms of the CPU time) is solving simultaneous equations, and the iteration cost with the filter method is about twice of the original method. The required iteration time for a 26×26 matrix with 1 zero eigenvalue solutions is 141 without acceleration and 25 with acceleration to get 5 solutions within 10^{-4} accuracy where λ_6/λ_5 equal to 1.046.

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